

PAC-Bayesian bounds for Principal Component Analysis in Hilbert spaces

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Abstract: Based on some new robust estimators of the covariance matrix, we propose stable versions of Principal Component Analysis (PCA) and we qualify it independently of the dimension of the ambient space. We first provide a robust estimator of the orthogonal projector on the largest eigenvectors of the covariance matrix. The behavior of such an estimator is related to the size of the gap in the spectrum of the covariance matrix and in particular a large gap is needed in order to get a good approximation. To avoid the assumption of a large eigengap in the spectrum of the covariance matrix we propose a robust version of PCA that consists in performing a smooth cut-off of the spectrum via a Lipschitz function. We provide bounds on the approximation error in terms of the operator norm and of the Frobenius norm.

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1. Introduction

Principal Component Analysis (PCA) is a classical tool for dimensionality reduction. The basic idea of PCA is to reduce the dimensionality of a dataset

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by projecting it into the space spanned by the directions of maximal variance, that are called its principal components. Since this set of directions lies in the space generated by the eigenvectors associated with the largest eigenvalues of the covariance matrix of the sample, the dimensionality reduction is achieved by projecting the dataset into the space spanned by these eigenvectors, which in the following we call *largest eigenvectors*.

Given $X \in \mathbb{R}^d$ a random vector distributed according to an unknown probability distribution $P \in \mathcal{M}_+^1(\mathbb{R}^d)$, the goal is to estimate the eigenvalues and eigenvectors of the covariance matrix of X

$$\Sigma = \mathbb{E}[(X - \mathbb{E}(X))(X - \mathbb{E}(X))^\top]$$

from an i.i.d. sample $X_1, \dots, X_n \in \mathbb{R}^d$ drawn according to P . Observe that in the case where the random vector X is centered (i.e. $\mathbb{E}[X] = 0$) the covariance matrix Σ is the Gram matrix

$$G = \mathbb{E}(XX^\top).$$

Many results concerning the Gram matrix estimate can be found in the literature, e.g. [7], [9], [8]. These results follow from the study of random matrix theory and use as an estimator of G the matrix obtained by replacing the unknown probability distribution P with the sample distribution $\frac{1}{n} \sum_{i=1}^n \delta_{X_i}$. In the following we call such an estimator *empirical Gram matrix*.

However, since the empirical Gram matrix, and consequently classical PCA, is sensitive to a heavy tailed sample distribution, several methods have been proposed to provide a stabler version of PCA, e.g. [1], [6]. In [1] the authors show that principal components of a data matrix can be recovered when part of the observations are contained in a low-dimensional space and the rest are arbitrarily corrupted. An alternative approach is proposed in [6] where, without assuming any geometrical assumption on the data, Minsker proposes a robust estimator of the Gram matrix, based on the geometric median. Such an estimator is used to provide non-asymptotic dimension-independent results concerning PCA.

We use the robust estimator \hat{G} proposed in [2] to describe a new approach that qualifies the stability of PCA independently of the dimension of the ambient space. Taking advantage of the fact that they are independent of the dimension, the results can be extended to the infinite-dimensional setting of separable Hilbert spaces and thus to kernel-PCA.

Results on PCA in Hilbert spaces can be found in Koltchinskii and Lounici [4], [5]. The authors study the problem of estimating the spectral projectors of the covariance operator by their empirical counterpart in the case of Gaussian centered random vectors, based on the bounds obtained in [3], and in the setting where both the sample size n and the trace of the covariance operator are large.

The paper is organized as follows. In section 2 we discuss some preliminary results presented in [2] on a robust estimator \hat{G} of the Gram matrix. In section 3

we prove that each eigenvalue $\hat{\lambda}_i$ of \hat{G} is a robust estimator of the corresponding eigenvalue of the Gram matrix. As a consequence, the orthogonal projector on the largest eigenvectors of G can be estimated by the projector on the largest eigenvectors of \hat{G} , providing a first version of robust PCA, as shown in section 4. The behavior of this estimator is related to the size of the gap in the spectrum of the Gram matrix and more precisely it is necessary to have a large eigengap in order to get a good approximation (Proposition 4.1). To avoid the assumption of a large gap in the spectrum of G we propose in section 5 another version of robust PCA which consists in performing a smooth cut-off of the spectrum of the Gram matrix via a Lipschitz function. We provide bounds on the approximation error, in terms of the operator norm (Proposition 5.2) and of the Frobenius norm (Proposition 5.3), that replace the size of the eigengap by the inverse of the Lipschitz constant of the cut-off function.

2. Preliminaries

In this section we discuss some results presented in [2] concerning the construction of a robust estimator of the Gram matrix. The idea is to use some PAC-Bayesian inequalities, linked to Gaussian perturbations, to first construct a confidence region for the quadratic form $\theta^\top G \theta$ and then to define a robust estimator for such a quantity. From a theoretical point of view we can consider any quadratic form belonging to the confidence interval obtained for $\theta^\top G \theta$. However from an algorithmic point of view, these constraints are imposed only for a finite number of directions. More precisely, we consider a symmetric matrix Q that satisfies the constraints for any θ in a finite δ -net of the unit sphere $\mathbb{S}_d = \{\theta \in \mathbb{R}^d, \|\theta\| = 1\}$. The construction of such an estimator is based on the computation of a convex optimization algorithm.

We first introduce some notation. Let, as in the introduction, $X \in \mathbb{R}^d$ be a random vector of law $P \in \mathcal{M}_+^1(\mathbb{R}^d)$. Let $a > 0$ and let

$$K = 1 + \left\lceil a^{-1} \log \left(\frac{n}{72(2+c)\kappa^{1/2}} \right) \right\rceil$$

where $c = \frac{15}{8 \log(2)(\sqrt{2}-1)} \exp\left(\frac{1+2\sqrt{2}}{2}\right)$ and

$$\kappa = \sup_{\substack{\theta \in \mathbb{R}^d \\ \mathbb{E}(\langle \theta, X \rangle^2) > 0}} \frac{\mathbb{E}(\langle \theta, X \rangle^4)}{\mathbb{E}(\langle \theta, X \rangle^2)^2}.$$

Let $s_4^2 = \mathbb{E}(\|X\|^4)^{1/2}$ and let $\sigma \in]0, s_4^2]$ be a threshold. We put

$$B_*(t) = \begin{cases} \frac{n^{-1/2} \zeta(\max\{t, \sigma\})}{1 - 4n^{-1/2} \zeta(\max\{t, \sigma\})} & [6 + (\kappa - 1)^{-1}] \zeta(\max\{t, \sigma\}) \leq \sqrt{n} \\ +\infty & \text{otherwise} \end{cases}$$

where

$$\begin{aligned} \zeta(t) = & \sqrt{2(\kappa - 1) \left(\frac{(2 + 3c) s_4^2}{4(2 + c)\kappa^{1/2}t} + \log(K/\epsilon) \right) \cosh(a/4)} \\ & + \sqrt{\frac{2(2 + c)\kappa^{1/2} s_4^2}{t} \cosh(a/2)}. \end{aligned} \quad (2.1)$$

The following proposition holds true.

Proposition 2.1. ([2]) *Let us assume that $8\zeta(\sigma) \leq \sqrt{n}$, $\sigma \leq s_4^2$ and that $\kappa \geq 3/2$. With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$,*

$$\begin{aligned} \left| \max\{\theta^\top Q\theta, \sigma\} - \max\{\theta^\top G\theta, \sigma\} \right| &\leq 2 \max\{\theta^\top G\theta, \sigma\} B_*(\theta^\top G\theta) + 5\delta \|G\|_F, \\ \left| \max\{\theta^\top Q\theta, \sigma\} - \max\{\theta^\top G\theta, \sigma\} \right| &\leq 2 \max\{\theta^\top Q\theta, \sigma\} B_*(\min\{\theta^\top Q\theta, s_4^2\}) \\ &\quad + 5\delta \|G\|_F. \end{aligned}$$

We recall that, given $M \in M_d(\mathbb{R})$ a symmetric $d \times d$ matrix, the Frobenius norm of M is defined as

$$\|M\|_F^2 = \text{Tr}(M^\top M)$$

and that $\|M\|_\infty \leq \|M\|_F$.

Observe that we assume that the threshold σ is such that $8\zeta(\sigma) \leq \sqrt{n}$ in order to have a meaningful bound. Indeed, in this case $B_*(t) < +\infty$, provided that $\kappa \geq 3/2$.

However, since we do not know whether Q is non-negative, we can decompose it in its positive and negative parts so that $Q = Q_+ - Q_-$ and consider as an estimator $\hat{G} = Q_+$. We deduce the following result.

Proposition 2.2. ([2]) *Let us assume that $8\zeta(\sigma) \leq \sqrt{n}$, $\sigma \leq s_4^2$ and that $\kappa \geq 3/2$. With probability at least $1 - 2\epsilon$, for any $\theta \in \mathbb{S}_d$,*

$$\begin{aligned} \left| \max\{\theta^\top \hat{G}\theta, \sigma\} - \max\{\theta^\top G\theta, \sigma\} \right| &\leq 2 \max\{\theta^\top G\theta, \sigma\} B_*(\theta^\top G\theta) + 7\delta \|G\|_F, \\ \left| \max\{\theta^\top \hat{G}\theta, \sigma\} - \max\{\theta^\top G\theta, \sigma\} \right| &\leq 2 \max\{\theta^\top \hat{G}\theta, \sigma\} B_*(\min\{\theta^\top \hat{G}\theta, s_4^2\}) \\ &\quad + 7\delta \|G\|_F. \end{aligned}$$

3. Estimate of the eigenvalues

Denote by $\lambda_1 \geq \dots \geq \lambda_d$ the eigenvalues of G and by p_1, \dots, p_d a corresponding orthonormal basis eigenvectors, so that $\lambda_i = p_i^\top G p_i$.

Similarly, let $\hat{\lambda}_1 \geq \dots \geq \hat{\lambda}_d$ be the eigenvalues of \hat{G} and q_1, \dots, q_d a corresponding orthonormal basis of eigenvectors.

In this section we prove that each eigenvalue of \hat{G} is a robust estimator of the corresponding eigenvalue of the Gram matrix.

Proposition 3.1. *Let us assume that $8\zeta(\sigma) \leq \sqrt{n}$, $\sigma \leq s_4^2$ and that $\kappa \geq 3/2$. With probability at least $1-2\epsilon$, for any $i = 1, \dots, d$, the two following inequalities hold together*

$$\begin{aligned} |\max\{\lambda_i, \sigma\} - \max\{\widehat{\lambda}_i, \sigma\}| &\leq 2 \max\{\lambda_i, \sigma\} B_*(\lambda_i) + 5\delta \|G\|_F, \\ |\max\{\lambda_i, \sigma\} - \max\{\widehat{\lambda}_i, \sigma\}| &\leq 2 \max\{\widehat{\lambda}_i, \sigma\} B_*(\min\{\widehat{\lambda}_i, s_4^2\}) + 5\delta \|G\|_F. \end{aligned}$$

Consequently,

$$\begin{aligned} |\lambda_i - \widehat{\lambda}_i| &\leq 2 \max\{\lambda_i, \sigma\} B_*(\lambda_i) + 5\delta \|G\|_F + \sigma, \\ |\lambda_i - \widehat{\lambda}_i| &\leq 2 \max\{\widehat{\lambda}_i, \sigma\} B_*(\min\{\widehat{\lambda}_i, s_4^2\}) + 5\delta \|G\|_F + \sigma. \end{aligned}$$

Proof. We observe that, for any $i \in \{1, \dots, d\}$, the vector space

$$\mathbf{span}\{q_1, \dots, q_{i-1}\}^\perp \cap \mathbf{span}\{p_1, \dots, p_i\} \subset \mathbb{R}^d$$

is of dimension at least 1, so that the set

$$V_i = \{\theta \in \mathbb{S}_d \mid \theta \in \mathbf{span}\{q_1, \dots, q_{i-1}\}^\perp \cap \mathbf{span}\{p_1, \dots, p_i\}\} \subset \mathbb{R}^d$$

is non-empty.

Indeed, putting $A = \mathbf{span}\{q_1, \dots, q_{i-1}\}^\perp$ and $B = \mathbf{span}\{p_1, \dots, p_i\}$, we see that $\dim(A \cap B) = \dim(A) + \dim(B) - \dim(A + B) \geq 1$, since $\dim(A + B) \leq \dim(\mathbb{R}^d) = d$ and $\dim(A) + \dim(B) = d + 1$. Hence, there exists $\theta_i \in V_i$ and for such a θ_i , we have $\theta_i^\top G \theta_i \geq \lambda_i$. It follows that

$$\begin{aligned} \max\{\lambda_i, \sigma\} &\leq \sup \{ \max\{\theta^\top G \theta, \sigma\} \mid \theta \in V_i \} \\ &\leq \sup \left\{ \max\{\theta^\top G \theta, \sigma\} \mid \theta \in \mathbb{S}_d, \theta \in \mathbf{span}\{q_1, \dots, q_{i-1}\}^\perp \right\}. \end{aligned}$$

Therefore, according to Proposition 2.1,

$$\begin{aligned} \max\{\lambda_i, \sigma\} (1 - 2B_*(\lambda_i)) &\leq \sup \left\{ \max\{\theta^\top G \theta, \sigma\} \mid \theta \in \mathbb{S}_d \cap \mathbf{span}\{q_1, \dots, q_{i-1}\}^\perp \right\} + 5\delta \|G\|_F \\ &\leq \max\{\widehat{\lambda}_i, \sigma\} + 5\delta \|G\|_F. \end{aligned}$$

In the same way,

$$\begin{aligned} \max\{\widehat{\lambda}_i, \sigma\} &\leq \sup \left\{ \max\{\theta^\top G \theta, \sigma\} \left(1 + 2B_*(\theta^\top G \theta) \right) \right. \\ &\quad \left. \mid \theta \in \mathbb{S}_d \cap \mathbf{span}\{p_1, \dots, p_{i-1}\}^\perp \right\} \\ &\quad + 5\delta \|G\|_F \\ &\leq \max\{\lambda_i, \sigma\} (1 + 2B_*(\lambda_i)) + 5\delta \|G\|_F, \end{aligned}$$

$$\begin{aligned}
 & \max\{\widehat{\lambda}_i, \sigma\} \left(1 - 2B_*(\min\{\widehat{\lambda}_i, s_4^2\})\right) \\
 & \leq \sup\left\{\max\{\theta^\top G\theta, \sigma\} \mid \theta \in \mathbb{S}_d \cap \mathbf{span}\{p_1, \dots, p_{i-1}\}^\perp\right\} + 5\delta\|G\|_F \\
 & \leq \max\{\lambda_i, \sigma\} + 5\delta\|G\|_F,
 \end{aligned}$$

and

$$\begin{aligned}
 \max\{\lambda_i, \sigma\} & \leq \sup\left\{\max\{\theta^\top Q\theta, \sigma\} \left(1 + 2B_*(\min\{\theta^\top Q\theta, s_4^2\})\right) \mid \right. \\
 & \quad \left. \theta \in \mathbb{S}_d \cap \mathbf{span}\{q_1, \dots, q_{i-1}\}^\perp\right\} + 5\delta\|G\|_F \\
 & \leq \max\{\widehat{\lambda}_i, \sigma\} \left(1 + 2B_*(\min\{\widehat{\lambda}_i, s_4^2\})\right) + 5\delta\|G\|_F.
 \end{aligned}$$

In all these inequalities we have used the fact that

$$\begin{aligned}
 t & \mapsto \max\{t, \sigma\} \left(1 - 2B_*(\min\{t, s_4^2\})\right) \\
 t & \mapsto \max\{t, \sigma\} \left(1 + 2B_*(\min\{t, s_4^2\})\right)
 \end{aligned}$$

are non-decreasing and that $\lambda_i \leq s_4^2$.

This proves the proposition for the eigenvalues of Q , and therefore also for their positive parts, that are the eigenvalues of $\widehat{G} = Q_+$.

To prove the second part of the proposition, it is sufficient to observe that

$$|\lambda_i - \widehat{\lambda}_i| \leq |\max\{\lambda_i, \sigma\} - \max\{\widehat{\lambda}_i, \sigma\}| + \sigma.$$

□

Given a threshold $\sigma \leq s_4^2$ such that $8\zeta(\sigma) \leq \sqrt{n}$, since the bound

$$F(t) = \max\{t, \sigma\} B_*(\min\{t, s_4^2\})$$

obtained in Proposition 3.1 is non-decreasing for any $t \in \mathbb{R}_+$, we get the following result:

Corollary 3.1. *Under the same assumptions as in Proposition 3.1, with probability at least $1 - 2\epsilon$, for any $i = 1, \dots, d$,*

$$\begin{aligned}
 |\lambda_i - \widehat{\lambda}_i| & \leq 2 \max\{\lambda_1, \sigma\} B_*(\lambda_1) + 5\delta\|G\|_F + \sigma, \\
 |\lambda_i - \widehat{\lambda}_i| & \leq 2 \max\{\widehat{\lambda}_1, \sigma\} B_*(\min\{\widehat{\lambda}_1, s_4^2\}) + 5\delta\|G\|_F + \sigma.
 \end{aligned}$$

In order to simplify notation, we define

$$B(t) = 2 \max\{t, \sigma\} B_*(\min\{t, s_4^2\}) + 7\delta\|G\|_F + \sigma. \quad (3.1)$$

Remark that, since B_* is non-increasing, F is non-decreasing and $B_*(t) \leq 1/4$, for any $a \in \mathbb{R}_+$, we have $B(t+a) \leq B(t) + a/2$.

4. Robust PCA

A method to determine the number of relevant components is based on the difference in magnitude between successive eigenvalues. In this section we study the projection on the r largest eigenvectors p_1, \dots, p_r of the Gram matrix, assuming that there is a gap in the spectrum of the Gram matrix, meaning that

$$\lambda_r - \lambda_{r+1} > 0. \quad (4.1)$$

We denote by Π_r the orthogonal projector on the r largest eigenvectors p_1, \dots, p_r of G and similarly by $\hat{\Pi}_r$ the orthogonal projector on the r largest eigenvectors q_1, \dots, q_r of its estimate \hat{G} .

Our goal is to provide a bound on the approximation $\|\Pi_r - \hat{\Pi}_r\|_\infty$ that does not depend explicitly on the dimension d of the ambient space.

Proposition 4.1. *With probability at least $1 - 2\epsilon$,*

$$\|\Pi_r - \hat{\Pi}_r\|_\infty \leq \frac{\sqrt{2r}}{\lambda_r - \lambda_{r+1}} B(\lambda_1)$$

where B is defined in equation (3.1) and λ_1 is the largest eigenvalue of the Gram matrix.

For the proof we refer to section 6.1.

We observe that the above proposition provides a bound on the approximation error $\|\Pi_r - \hat{\Pi}_r\|_\infty$ that does not depend explicitly on the dimension d of the ambient space, since B is dimension-free. However the result relates the quality of the approximation of the orthogonal projector Π_r by the robust estimator $\hat{\Pi}_r$ to the size of the spectral gap and in particular the larger the eigengap, the better the approximation is. A way to estimate the size of the eigengap is by using the eigenvalues of the robust estimator \hat{G} , since, according to Proposition 3.1, each eigenvalue of \hat{G} provides a good approximation of the corresponding eigenvalue of the Gram matrix.

5. Robust PCA with a smooth cut-off

In order to avoid the requirement of a large spectral gap, we can interpret the projector Π_r as a step function applied to the spectrum of the Gram matrix and consider to replace Π_r with a smooth cut-off of the eigenvalues of G via a Lipschitz function. More specifically, we have in mind to apply to the spectrum of G a Lipschitz function that takes the value one on the largest eigenvalues and the value zero on the smallest ones.

Let f be a Lipschitz function with Lipschitz constant $1/L$. We decompose the Gram matrix as

$$G = UDU^\top$$

where $D = \text{diag}(\lambda_1, \dots, \lambda_d) \in M_d(\mathbb{R})$ is the diagonal matrix whose entries are the eigenvalues of G and $U \in M_d(\mathbb{R})$ is the orthogonal matrix of eigenvectors of G . We define $f(G)$ as

$$f(G) = U \text{diag}\left(f(\lambda_1), \dots, f(\lambda_d)\right) U^\top$$

where, for any $i, j \in \{1, \dots, d\}$,

$$|f(\lambda_i) - f(\lambda_j)| \leq \frac{1}{L} |\lambda_i - \lambda_j|.$$

We provide some results on the estimate of $f(G)$, the image of the Gram matrix by the smooth cut-off f , in terms of the operator norm $\|\cdot\|_\infty$ and of the Frobenius norm $\|\cdot\|_F$. We start with a general result.

Proposition 5.1. *Let $M, M' \in M_d(\mathbb{R})$ be two symmetric matrices. We denote by μ_1, \dots, μ_d the eigenvalues of M related to the orthonormal basis of eigenvectors p_1, \dots, p_d and by μ'_1, \dots, μ'_d the eigenvalues of M' related to the orthonormal basis of eigenvectors q_1, \dots, q_d . We have*

$$\|M - M'\|_F^2 = \sum_{i,k=1}^d (\mu_i - \mu'_k)^2 \langle p_i, q_k \rangle^2. \quad (5.1)$$

Moreover, let f be a $1/L$ -Lipschitz function. We have

$$\|f(M) - f(M')\|_F \leq \frac{1}{L} \|M - M'\|_F. \quad (5.2)$$

For the proof we refer to section 6.2.

Let us now present the bound on the approximation error $\|f(G) - f(\hat{G})\|_\infty$ in terms of the operator norm.

Proposition 5.2. (Operator norm) *With probability at least $1 - 2\epsilon$, for any $1/L$ -Lipschitz function f ,*

$$\|f(G) - f(\hat{G})\|_\infty \leq \min_{r \in \{1, \dots, d\}} L^{-1} \left(B(\lambda_1) + \sqrt{4rB(\lambda_1)^2 + 2 \sum_{i=r+1}^d \lambda_i^2} \right),$$

where B is defined in equation (3.1) and $\lambda_1 \geq \dots \geq \lambda_d$ are the eigenvalues of G .

For the proof we refer to section 6.3.

Observe that with respect to the bound obtained in Proposition 4.1, we have replaced the inverse of the size of the gap with the Lipschitz constant. Moreover, in the case it exists a gap $\lambda_r - \lambda_{r+1} > 0$, there exists a Lipschitz function f such that $\Pi_r = f(G)$ and whose Lipschitz constant is exactly the inverse of the size

of the gap. Otherwise, if we want to use f with a better Lipschitz constant, we have to approximate Π_r with the smoother approximate projection $f(G)$.

Slightly changing the definition of the estimator we can obtain a bound for the approximation error in terms of the Frobenius norm. Instead of considering $\hat{G} = \sum_{i=1}^d \hat{\lambda}_i q_i q_i^\top$ we consider the matrix

$$\tilde{G} = \sum_{i=1}^d \tilde{\lambda}_i q_i q_i^\top$$

with eigenvectors q_1, \dots, q_d and eigenvalues

$$\tilde{\lambda}_i = \left[\hat{\lambda}_i - B(\hat{\lambda}_i) \right]_+$$

where we recall that B is defined in equation (3.1). We observe that, in the event of probability at least $1 - 2\epsilon$ described in Corollary 3.1, for any $i = 1, \dots, d$,

$$\tilde{\lambda}_i \leq \lambda_i.$$

According to Proposition 5.1, we first present a result on the approximation error $\|G - \tilde{G}\|_F$.

Proposition 5.3. (Frobenius norm) *With probability at least $1 - 2\epsilon$,*

$$\|G - \tilde{G}\|_F \leq \min_{r \in \{1, \dots, d\}} \sqrt{13rB(\lambda_1)^2 + 2 \sum_{i=r+1}^d \lambda_i^2},$$

where B is defined in equation (3.1) and $\lambda_1 \geq \dots \geq \lambda_d$ are the eigenvalues of G .

For the proof we refer to section 6.4.

To obtain a bound on $\|f(G) - f(\tilde{G})\|_F$ it is sufficient to combine the above proposition with Proposition 5.2.

Corollary 5.1. *With the same notation as in Proposition 5.3, with probability at least $1 - 2\epsilon$, for any $1/L$ -Lipschitz function f ,*

$$\|f(G) - f(\tilde{G})\|_F \leq \min_{r \in \{1, \dots, d\}} L^{-1} \sqrt{13rB(\lambda_1)^2 + 2 \sum_{i=r+1}^d \lambda_i^2}.$$

In the previous bounds, the optimal choice of the dimension parameter r depends on the distribution of the eigenvalues of the Gram matrix G . Nevertheless, it is possible to upper bound what happens when this distribution of eigenvalues is the worst possible.

Observe that

$$\sum_{i=r+1}^d \lambda_i^2 \leq \lambda_{r+1} \mathbf{Tr}(G)$$

and also $r\lambda_{r+1} \leq \mathbf{Tr}(G)$, so that

$$\sum_{i=r+1}^d \lambda_i^2 \leq r^{-1} \mathbf{Tr}(G)^2.$$

Hence, if we consider for example the case where the approximation error is evaluated in terms of the Frobenius norm, the worst case formulation of Corollary 5.1 is obtained choosing

$$r = \left\lceil \sqrt{2/13} \mathbf{Tr}(G) B(\lambda_1)^{-1} \right\rceil$$

and, in this case, it can be restated as follows.

Corollary 5.2. *With probability at least $1 - 2\epsilon$,*

$$\|f(G) - f(\tilde{G})\|_F \leq L^{-1} \sqrt{11 \mathbf{Tr}(G) B(\lambda_1) + 13 B(\lambda_1)^2}.$$

This proposition shows that the worst case speed is not slower than $n^{-1/4}$. We do not know whether this rate is optimal in the worst case. We could in the same way obtain a worst case corollary for Proposition 5.2.

6. Proofs

In this section we give the proofs of the results presented in the previous sections. More precisely, section 6.1 refers to Proposition 4.1, section 6.2 refers to Proposition 5.1, section 6.3 refers to Proposition 5.2 and section 6.4 refers to Proposition 5.3. We start with a technical lemma that will be useful in several proofs.

Lemma 6.1. *With probability at least $1 - 2\epsilon$, for any $k \in \{1, \dots, d\}$, the two inequalities hold together*

$$\sum_{i=1}^d (\lambda_i - \lambda_k)^2 \langle q_k, p_i \rangle^2 \leq 2B(\lambda_1)^2 \quad (6.1)$$

$$\sum_{i=1}^d (\lambda_i - \hat{\lambda}_k)^2 \langle q_k, p_i \rangle^2 \leq B(\lambda_1)^2, \quad (6.2)$$

where $B(t) = 2 \max\{t, \sigma\} B_*(\min\{t, s_4^2\}) + 7\delta \|G\|_F + \sigma$ is defined in equation (3.1).

Proof. We observe that,

$$\begin{aligned}\|G - \widehat{G}\|_\infty &= \max \left\{ \sup_{\theta \in \mathbb{S}_d} \theta^\top (G - \widehat{G})\theta, \sup_{\theta \in \mathbb{S}_d} \theta^\top (\widehat{G} - G)\theta \right\} \\ &= \sup_{\theta \in \mathbb{S}_d} |\theta^\top G\theta - \theta^\top \widehat{G}\theta| \\ &\leq \sup_{\theta \in \mathbb{S}_d} |\max\{\theta^\top G\theta, \sigma\} - \max\{\theta^\top \widehat{G}\theta, \sigma\}| + \sigma\end{aligned}$$

for any threshold $\sigma > 0$. Thus, by Proposition 2.2, with probability at least $1 - 2\epsilon$,

$$\sup_{\theta \in \mathbb{S}_d} \|G\theta - \widehat{G}\theta\| \leq B(\lambda_1).$$

To prove equation (6.2) it is sufficient to observe that, since

$$\|G\theta - \widehat{G}\theta\| = \left\| \sum_{i,j=1}^d (\lambda_i - \widehat{\lambda}_j) \langle \theta, q_j \rangle \langle p_i, q_j \rangle p_i \right\|$$

choosing $\theta = q_k$, with $k \in \{1, \dots, d\}$,

$$\|Gq_k - \widehat{G}q_k\|^2 = \sum_{i=1}^d (\lambda_i - \widehat{\lambda}_k)^2 \langle q_k, p_i \rangle^2.$$

On the other hand, to prove equation (6.1), we observe that

$$\begin{aligned}\|G\theta - \widehat{G}\theta\| &= \left\| \sum_{i=1}^d \lambda_i \langle \theta, p_i \rangle p_i - \sum_{i=1}^d \widehat{\lambda}_i \langle \theta, q_i \rangle q_i \right\| \\ &= \left\| \sum_{i=1}^d \lambda_i (\langle \theta, p_i \rangle p_i - \langle \theta, q_i \rangle q_i) - \sum_{i=1}^d (\widehat{\lambda}_i - \lambda_i) \langle \theta, q_i \rangle q_i \right\| \\ &\geq \left\| \sum_{i=1}^d \lambda_i (\langle \theta, p_i \rangle p_i - \langle \theta, q_i \rangle q_i) \right\| - \left\| \sum_{i=1}^d (\widehat{\lambda}_i - \lambda_i) \langle \theta, q_i \rangle q_i \right\|\end{aligned}$$

where, by Corollary 3.1,

$$\left\| \sum_{i=1}^d (\widehat{\lambda}_i - \lambda_i) \langle \theta, q_i \rangle q_i \right\|^2 = \sum_{i=1}^d (\widehat{\lambda}_i - \lambda_i)^2 \langle \theta, q_i \rangle^2 \leq B(\lambda_1)^2.$$

Choosing again $\theta = q_k$, for $k \in \{1, \dots, d\}$, we get

$$\begin{aligned}
 \left\| \sum_{i=1}^d \lambda_i (\langle q_k, p_i \rangle p_i - \langle q_k, q_i \rangle q_i) \right\|^2 &= \left\| \sum_{i,j=1}^d (\lambda_i - \lambda_j) \langle q_k, q_j \rangle \langle q_j, p_i \rangle p_i \right\|^2 \\
 &= \left\| \sum_{i=1}^d (\lambda_i - \lambda_k) \langle q_k, p_i \rangle p_i \right\|^2 \\
 &= \sum_{i=1}^d (\lambda_i - \lambda_k)^2 \langle q_k, p_i \rangle^2,
 \end{aligned}$$

which concludes the proof. \square

6.1. Proof of Proposition 4.1

Since Π_r and $\widehat{\Pi}_r$ have the same rank, we can write

$$\|\Pi_r - \widehat{\Pi}_r\|_\infty = \sup_{\substack{\theta \in \mathbb{S}_d \\ \theta \in \mathbf{Im}(\widehat{\Pi}_r)}} \|\Pi_r \theta - \widehat{\Pi}_r \theta\|$$

as shown in Lemma A.5 in Appendix A. Moreover, for any $\theta \in \mathbf{Im}(\widehat{\Pi}_r) \cap \mathbb{S}_d$, we observe that

$$\begin{aligned}
 \|\Pi_r \theta - \widehat{\Pi}_r \theta\|^2 &= \|\Pi_r \theta - \theta\|^2 \\
 &= \left\| \sum_{i=1}^r \langle \theta, p_i \rangle p_i - \sum_{i=1}^d \langle \theta, p_i \rangle p_i \right\|^2 \\
 &= \sum_{i=r+1}^d \langle \theta, p_i \rangle^2.
 \end{aligned}$$

Since any $\theta \in \mathbf{Im}(\widehat{\Pi}_r)$ can be written as $\theta = \sum_{k=1}^r \langle \theta, q_k \rangle q_k$ with $\sum_{k=1}^r \langle \theta, q_k \rangle^2 = 1$, then

$$\|\Pi_r \theta - \widehat{\Pi}_r \theta\|^2 = \sum_{i=r+1}^d \left(\sum_{k=1}^r \langle \theta, q_k \rangle \langle q_k, p_i \rangle \right)^2.$$

Hence, by the Cauchy-Schwarz inequality, we get

$$\|\Pi_r \theta - \widehat{\Pi}_r \theta\|^2 \leq \sum_{i=r+1}^d \left(\sum_{k=1}^r \langle \theta, q_k \rangle^2 \right) \left(\sum_{k=1}^r \langle q_k, p_i \rangle^2 \right) \quad (6.3)$$

$$= \sum_{k=1}^r \sum_{i=r+1}^d \langle q_k, p_i \rangle^2. \quad (6.4)$$

Moreover, for any $k \in \{1, \dots, r\}$, we have

$$\begin{aligned} \sum_{i=r+1}^d (\lambda_k - \lambda_i)^2 \langle q_k, p_i \rangle^2 &\geq \sum_{i=r+1}^d (\lambda_r - \lambda_i)^2 \langle q_k, p_i \rangle^2 \\ &\geq (\lambda_r - \lambda_{r+1})^2 \sum_{i=r+1}^d \langle q_k, p_i \rangle^2. \end{aligned}$$

Then, by Lemma 6.1, with probability at least $1 - 2\epsilon$,

$$(\lambda_r - \lambda_{r+1})^2 \sum_{i=r+1}^d \langle q_k, p_i \rangle^2 \leq 2B(\lambda_1)^2.$$

Applying the above inequality to equation (6.4) we conclude the proof.

6.2. Proof of Proposition 5.1

Since $\{p_i\}_{i=1}^d$ is an orthonormal basis of eigenvectors of M and $\{\mu_i\}_{i=1}^d$ the corresponding eigenvalues, we can write M as

$$M = \sum_{i=1}^d \mu_i p_i p_i^\top.$$

Similarly,

$$M' = \sum_{i=1}^d \mu'_i q_i q_i^\top.$$

Our goal is to evaluate $\|M - M'\|_F$ where, by definition,

$$\begin{aligned} M - M' &= \sum_{i=1}^d \mu_i p_i p_i^\top - \sum_{k=1}^d \mu'_k q_k q_k^\top \\ &= \sum_{i,k=1}^d (\mu_i - \mu'_k) \langle p_i, q_k \rangle q_k p_i^\top. \end{aligned}$$

We observe that $M - M'$ is a symmetric matrix and its Frobenius norm is

$$\|M - M'\|_F^2 = \mathbf{Tr}((M - M')^\top (M - M')),$$

where

$$(M - M')^\top (M - M') = \sum_{i,j,k=1}^d (\mu_i - \mu'_k)(\mu_i - \mu'_j) \langle p_i, q_k \rangle \langle p_i, q_j \rangle q_k q_j^\top.$$

Considering that $\mathbf{Tr}(q_k q_j^\top) = \delta_{jk}$, we conclude that

$$\begin{aligned}\|M - M'\|_F^2 &= \sum_{i,j,k=1}^d (\mu_i - \mu'_k)(\mu_i - \mu'_j) \langle p_i, q_k \rangle \langle p_i, q_j \rangle \delta_{jk} \\ &= \sum_{i,k=1}^d (\mu_i - \mu'_k)^2 \langle p_i, q_k \rangle^2.\end{aligned}$$

To prove the second part of the result, it is sufficient to observe that using twice equation (5.1). Indeed

$$\begin{aligned}\|f(M) - f(M')\|_F^2 &= \sum_{i,k=1}^d (f(\mu_i) - f(\mu'_k))^2 \langle p_i, q_k \rangle^2 \\ &\leq \frac{1}{L^2} \sum_{i,k=1}^d (\mu_i - \mu'_k)^2 \langle p_i, q_k \rangle^2 = \frac{1}{L^2} \|M - M'\|_F^2.\end{aligned}$$

6.3. Proof of Proposition 5.2

In all this proof, we will assume that the event of probability at least $1 - 2\epsilon$ described in Proposition 3.1 holds true. Let $H \in M_d(\mathbb{R})$ be the matrix defined as

$$H = \sum_{k=1}^d \lambda_k q_k q_k^\top.$$

We observe that

$$\|f(G) - f(\widehat{G})\|_\infty \leq \|f(G) - f(H)\|_\infty + \|f(H) - f(\widehat{G})\|_\infty$$

and we look separately at the two terms. By definition of operator norm, we have

$$\begin{aligned}\|f(H) - f(\widehat{G})\|_\infty^2 &= \sup_{\theta \in \mathbb{S}_d} \|f(H)\theta - f(\widehat{G})\theta\|^2 \\ &= \sup_{\theta \in \mathbb{S}_d} \left\| \sum_{k=1}^d (f(\lambda_k) - f(\widehat{\lambda}_k)) \langle \theta, q_k \rangle q_k \right\|^2 \\ &= \sup_{\theta \in \mathbb{S}_d} \sum_{k=1}^d (f(\lambda_k) - f(\widehat{\lambda}_k))^2 \langle \theta, q_k \rangle^2.\end{aligned}$$

Since the function f is $1/L$ -Lipschitz, we get

$$\|f(H) - f(\widehat{G})\|_\infty^2 \leq L^{-2} \sup_{\theta \in \mathbb{S}_d} \sum_{k=1}^d (\lambda_k - \widehat{\lambda}_k)^2 \langle \theta, q_k \rangle^2$$

and then, applying Corollary 3.1, with probability at least $1 - 2\epsilon$, we obtain

$$\|f(H) - f(\widehat{G})\|_\infty^2 \leq L^{-2} B(\lambda_1)^2.$$

On the other hand, we have

$$\begin{aligned} \|f(G) - f(H)\|_\infty &\leq \|f(G) - f(H)\|_F \\ &\leq \frac{1}{L} \|G - H\|_F, \end{aligned}$$

as shown in equation (5.2). Hence, according to Proposition 5.1, we get

$$\|f(G) - f(H)\|_\infty^2 \leq \frac{1}{L^2} \sum_{i,k=1}^d (\lambda_i - \lambda_k)^2 \langle p_i, q_k \rangle^2$$

where, for any r ,

$$\sum_{i,k=1}^d (\lambda_i - \lambda_k)^2 \langle p_i, q_k \rangle^2 \leq \left(\sum_{i=1}^r \sum_{k=1}^d + \sum_{i=1}^d \sum_{k=1}^r + \sum_{i,k=r+1}^d \right) (\lambda_i - \lambda_k)^2 \langle p_i, q_k \rangle^2.$$

Since $\lambda_i \geq 0$, for any $i \in \{1, \dots, d\}$, we get

$$\sum_{i,k=r+1}^d (\lambda_i - \lambda_k)^2 \langle p_i, q_k \rangle^2 \leq 2 \sum_{i=r+1}^d \lambda_i^2.$$

Moreover, by Lemma 6.1, we have

$$\sum_{k=1}^r \sum_{i=1}^d (\lambda_i - \lambda_k)^2 \langle p_i, q_k \rangle^2 \leq 2rB(\lambda_1)^2$$

and since the same bound also holds for

$$\sum_{i=1}^r \sum_{k=1}^d (\lambda_i - \lambda_k)^2 \langle p_i, q_k \rangle^2,$$

we conclude the proof.

6.4. Proof of Proposition 5.3

During the whole proof, we will assume that the event of probability at least $1 - 2\epsilon$ described in Proposition 3.1 is realized. According to Proposition 5.1, we have

$$\|G - \widetilde{G}\|_F^2 = \sum_{i,k=1}^d (\lambda_i - \widetilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2,$$

where

$$\sum_{i,k=1}^d (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2 \leq \left(\sum_{i=1}^r \sum_{k=1}^d + \sum_{k=1}^r \sum_{i=1}^d + \sum_{i,k=r+1}^d \right) (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2.$$

Since, by definition, $\tilde{\lambda}_i \leq \lambda_i$, it follows that

$$\begin{aligned} \sum_{i,k=r+1}^d (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2 &\leq \sum_{i,k=r+1}^d (\lambda_i^2 + \tilde{\lambda}_k^2) \langle p_i, q_k \rangle^2 \\ &\leq 2 \sum_{i=r+1}^d \lambda_i^2. \end{aligned}$$

Furthermore, we observe that

$$\sum_{k=1}^r \sum_{i=1}^d (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2 \leq 2 \sum_{k=1}^r \sum_{i=1}^d (\lambda_i - \hat{\lambda}_k)^2 \langle p_i, q_k \rangle^2 + 2 \sum_{k=1}^r \sum_{i=1}^d B(\hat{\lambda}_k)^2 \langle p_i, q_k \rangle^2,$$

where, by Lemma 6.1,

$$\sum_{k=1}^r \sum_{i=1}^d (\lambda_i - \hat{\lambda}_k)^2 \langle p_i, q_k \rangle^2 \leq rB(\lambda_1)^2.$$

and $B(\hat{\lambda}_k) \leq B(\hat{\lambda}_1)$. We have then proved that

$$\sum_{k=1}^r \sum_{i=1}^d (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2 \leq 2rB(\lambda_1)^2 + 2rB(\hat{\lambda}_1)^2.$$

Applying Corollary 3.1 and using the fact that $B(t+a) \leq B(t) + a/2$, as explained after equation (3.1), we deduce that

$$B(\hat{\lambda}_1) \leq B[\lambda_1 + B(\lambda_1)] \leq 3B(\lambda_1)/2.$$

This proves that

$$\sum_{k=1}^r \sum_{i=1}^d (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2 \leq 2r [B(\lambda_1)^2 + 9B(\lambda_1)^2/4] = 13rB(\lambda_1)^2/2.$$

Considering that the same bound holds for

$$\sum_{i=1}^r \sum_{k=1}^d (\lambda_i - \tilde{\lambda}_k)^2 \langle p_i, q_k \rangle^2,$$

we conclude the proof.

Appendix A: Orthogonal Projectors

In this appendix we introduce some results on orthogonal projectors.

Let $P, Q : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be two orthogonal projectors. We denote by \mathbb{S}_d the unit sphere of \mathbb{R}^d . By definition,

$$\|P - Q\|_\infty = \sup_{x \in \mathbb{S}_d} \|Px - Qx\|$$

where, without loss of generality, we can take the supremum over the normalized eigenvectors of $P - Q$.

A good way to describe the geometry of $P - Q$ is to consider the eigenvectors of $P + Q$.

Lemma A.1. *Let $x \in \mathbb{S}_d$ be an eigenvector of $P + Q$ with eigenvalue λ .*

1. *In the case when $\lambda = 0$, then $Px = Qx = 0$, so that $x \in \ker(P) \cap \ker(Q)$;*
2. *in the case when $\lambda = 1$, then $PQx = QPx = 0$, so that*

$$x \in \ker(P) \cap \text{Im}(Q) \oplus \text{Im}(P) \cap \ker(Q);$$

3. *in the case when $\lambda = 2$, then $x = Px = Qx$, so that $x \in \text{Im}(P) \cap \text{Im}(Q)$;*
4. *otherwise $\lambda \in]0, 1[\cup]1, 2[$,*

$$(P - Q)^2 x = (2 - \lambda)\lambda x \neq 0,$$

so that $(P - Q)x \neq 0$. Moreover

$$(P + Q)(P - Q)x = (2 - \lambda)(P - Q)x,$$

so that $(P - Q)x$ is an eigenvector of $P + Q$ with eigenvalue $2 - \lambda$. Moreover

$$0 < \|Px\| = \|Qx\| < \|x\|,$$

$x - Px \neq 0$, and $(Px, x - Px)$ is an orthogonal basis of $\text{span}\{x, (P - Q)x\}$.

Proof. The operator $P + Q$ is symmetric, positive semi-definite, and $\|P + Q\| \leq 2$, so that there is a basis of eigenvectors and all eigenvalues are in the interval $[0, 2]$.

In case 1, $0 = \langle Px + Qx, x \rangle = \|Px\|^2 + \|Qx\|^2$, so that $Px = Qx = 0$.

In case 2, $PQx = P(x - Px) = 0$ and similarly $QPx = Q(x - Qx) = 0$.

In case 3,

$$\|Px\|^2 + \|Qx\|^2 = \langle (P + Q)x, x \rangle = 2\langle x, x \rangle = \|Px\|^2 + \|x - Px\|^2 + \|Qx\|^2 + \|x - Qx\|^2,$$

so that $\|x - Px\| = \|x - Qx\| = 0$.

In case 4, remark that

$$PQx = P(\lambda x - Px) = (\lambda - 1)Px$$

and similarly $QP x = Q(\lambda x - Qx) = (\lambda - 1)Qx$. Consequently

$$(P - Q)(P - Q)x = (P - QP - PQ + Q)x = (2 - \lambda)(P + Q)x = (2 - \lambda)\lambda x \neq 0,$$

so that $(P - Q)x \neq 0$. Moreover

$$(P + Q)(P - Q)x = (P - PQ + QP - Q)x = (2 - \lambda)(P - Q)x.$$

Therefore $(P - Q)x$ is an eigenvector of $P + Q$ with eigenvalue $2 - \lambda \neq \lambda$, so that $\langle x, (P - Q)x \rangle = 0$, since $P + Q$ is symmetric. As $\langle x, (P - Q)x \rangle = \|Px\|^2 - \|Qx\|^2$, this proves that $\|Px\| = \|Qx\|$. Since $(P + Q)x = \lambda x \neq 0$, necessarily $\|Px\| = \|Qx\| > 0$. Observe now that

$$\|Px\|^2 = \frac{1}{2}(\|Px\|^2 + \|Qx\|^2) = \frac{1}{2}\langle x, (P + Q)x \rangle = \frac{\lambda}{2}\|x\|^2 < \|x\|^2.$$

Therefore $\|x - Px\|^2 = \|x\|^2 - \|Px\|^2 > 0$, proving that $x - Px \neq 0$. Similarly, since P and Q play symmetric roles, $\|Qx\| < \|x\|$ and $x - Qx \neq 0$.

As P is an orthogonal projector, $(Px, x - Px)$ is an orthogonal pair of non-zero vectors. Moreover

$$x = x - Px + Px \in \mathbf{span}\{Px, x - Px\}$$

and

$$(P - Q)x = 2Px - \lambda x = (2 - \lambda)Px - \lambda(x - Px) \in \mathbf{span}\{Px, x - Px\}$$

therefore, $(Px, x - Px)$ is an orthogonal basis of $\mathbf{span}\{x, (P - Q)x\}$. \square

Lemma A.2. *There is an orthonormal basis $(x_i)_{i=1}^d$ of eigenvectors of $P + Q$ with corresponding eigenvalues $\{\lambda_i, i = 1, \dots, d\}$ and indices $2m \leq p \leq q \leq s$, such that*

1. $\lambda_i \in]1, 2[$, if $1 \leq i \leq m$,
2. $\lambda_{m+i} = 2 - \lambda_i$, if $1 \leq i \leq m$, and $x_{m+i} = \|(P - Q)x_i\|^{-1}(P - Q)x_i$,
3. $x_{2m+1}, \dots, x_p \in (\mathbf{Im}(P) \cap \mathbf{ker}(Q))$, and $\lambda_{2m+1} = \dots = \lambda_p = 1$,
4. $x_{p+1}, \dots, x_q \in (\mathbf{Im}(Q) \cap \mathbf{ker}(P))$, and $\lambda_{p+1} = \dots = \lambda_q = 1$,
5. $x_{q+1}, \dots, x_s \in \mathbf{Im}(P) \cap \mathbf{Im}(Q)$, and $\lambda_{q+1} = \dots = \lambda_s = 2$,
6. $x_{s+1}, \dots, x_d \in \mathbf{ker}(P) \cap \mathbf{ker}(Q)$, and $\lambda_{s+1} = \dots = \lambda_d = 0$.

Proof. There exists a basis of eigenvectors of $P + Q$ (as already explained at the beginning of proof of Lemma A.1). From the previous lemma, we learn that all eigenvectors in the kernel of $P + Q$ are in $\mathbf{ker}(P) \cap \mathbf{ker}(Q)$, as on the other hand obviously $\mathbf{ker}(P) \cap \mathbf{ker}(Q) \subset \mathbf{ker}(P + Q)$ we get that

$$\mathbf{ker}(P + Q) = \mathbf{ker}(P) \cap \mathbf{ker}(Q).$$

In the same way the previous lemma proves that the eigenspace corresponding to the eigenvalue 2 is equal to $\mathbf{Im}(P) \cap \mathbf{Im}(Q)$. It also proves that the eigenspace corresponding to the eigenvalue 1 is included in and consequently is equal to

$(\mathbf{Im}(P) \cap \mathbf{ker}(Q)) \oplus (\mathbf{ker}(P) \cap \mathbf{Im}(Q))$, so that we can form an orthonormal basis of this eigenspace by taking the union of an orthonormal basis of $\mathbf{Im}(P) \cap \mathbf{ker}(Q)$ and an orthonormal basis of $\mathbf{ker}(P) \cap \mathbf{Im}(Q)$.

Consider now an eigenspace corresponding to an eigenvalue $\lambda \in]0, 1[\cup]1, 2[$ and let x, y be two orthonormal eigenvectors in this eigenspace. Remark that (still from the previous lemma)

$$\langle (P - Q)x, (P - Q)y \rangle = \langle (P - Q)^2 x, y \rangle = (2 - \lambda)\lambda \langle x, y \rangle = 0.$$

Therefore, if x_1, \dots, x_k is an orthonormal basis of the eigenspace V_λ corresponding to the eigenvalue λ , then $(P - Q)x_1, \dots, (P - Q)x_k$ is an orthogonal system in $V_{2-\lambda}$. If this system was not spanning $V_{2-\lambda}$, we could add to it an orthogonal unit vector $y_{k+1} \in V_{2-\lambda}$ so that $x_1, \dots, x_k, (P - Q)y_{k+1}$ would be an orthogonal set of non-zero vectors in V_λ , which would contradict the fact that x_1, \dots, x_k was supposed to be an orthonormal basis of V_λ . Therefore,

$$\left(\|(P - Q)x_i\|^{-1} (P - Q)x_i, 1 \leq i \leq k \right)$$

is an orthonormal basis of $V_{2-\lambda}$. Doing this construction for all the eigenspaces V_λ such that $\lambda \in]0, 1[$ achieves the construction of the orthonormal basis described in the lemma. \square

Lemma A.3. *Consider the orthonormal basis of the previous lemma. The set of vectors*

$$(Px_1, \dots, Px_m, x_{2m+1}, \dots, x_p, x_{q+1}, \dots, x_s)$$

is an orthogonal basis of $\mathbf{Im}(P)$. The set of vectors

$$(Qx_1, \dots, Qx_m, x_{p+1}, \dots, x_q, x_{q+1}, \dots, x_s)$$

is an orthogonal basis of $\mathbf{Im}(Q)$.

Proof. According to Lemma A.1, $(Px_i, x_i - Px_i)$ is an orthogonal basis of $\mathbf{span}\{x_i, x_{m+i}\}$, so that

$$(Px_1, \dots, Px_m, x_1 - Px_1, \dots, x_m - Px_m, x_{2m+1}, \dots, x_d)$$

is another orthogonal basis of \mathbb{R}^d . Each vector of this basis is either in $\mathbf{Im}(P)$ or in $\mathbf{ker}(P)$ and more precisely

$$\begin{aligned} Px_1, \dots, Px_m, x_{2m+1}, \dots, x_p, x_{q+1}, \dots, x_s &\in \mathbf{Im}(P), \\ x_1 - Px_1, \dots, x_m - Px_m, x_{p+1}, \dots, x_q, x_{s+1}, \dots, x_d &\in \mathbf{ker}(P). \end{aligned}$$

This proves the claim of the lemma concerning P . Since P and Q play symmetric roles, this proves also the claim concerning Q , *mutatis mutandis*. \square

Lemma A.4. *The projectors P and Q have the same rank if and only if*

$$p - 2m = q - p.$$

Lemma A.5. Assume that $\text{rk}(P) = \text{rk}(Q)$. Then

$$\|P - Q\|_\infty = \sup_{\theta \in \mathbf{Im}(Q) \cap \mathbb{S}_d} \|(P - Q)\theta\|.$$

Proof. As $P - Q$ is a symmetric operator, we have

$$\begin{aligned} \sup_{\theta \in \mathbb{S}_d} \|(P - Q)\theta\|^2 &= \sup \left\{ \langle (P - Q)^2 \theta, \theta \rangle \mid \theta \in \mathbb{S}_d \right\} \\ &= \sup \left\{ \langle (P - Q)^2 \theta, \theta \rangle \mid \theta \in \mathbb{S}_d \text{ is an eigenvector of } (P - Q)^2 \right\}. \end{aligned}$$

Remark that the basis described in Lemma A.2 is also a basis of eigenvectors of $(P - Q)^2$. More precisely, according to Lemma A.1

$$\begin{aligned} (P - Q)^2 x_i &= \lambda_i(2 - \lambda_i)x_i, & 1 \leq i \leq m, \\ (P - Q)^2 x_{m+i} &= \lambda_i(2 - \lambda_i)x_{m+i}, & 1 \leq i \leq m, \\ (P - Q)^2 x_i &= x_i, & 2m < i \leq q, \\ (P - Q)^2 x_i &= 0, & q < i \leq d. \end{aligned}$$

If $q - 2m > 0$, then $\|P - Q\|_\infty = 1$, and $q - p > 0$, according to Lemma A.4, so that $\|(P - Q)x_{p+1}\| = 1$, where $x_{p+1} \in \mathbf{Im}(Q)$. If $q = 2m$ and $m > 0$, there is $i \in \{1, \dots, m\}$ such that $\|P - Q\|_\infty^2 = \lambda_i(2 - \lambda_i)$. Since x_i and x_{m+i} are two eigenvectors of $(P - Q)^2$ corresponding to this eigenvalue, all the non-zero vectors in $\text{span}\{x_i, x_{m+i}\}$ (including Qx_i) are also eigenvectors of the same eigenspace. Consequently $(P - Q)^2 Qx_i = \lambda_i(2 - \lambda_i)Qx_i$, proving that

$$\left\| (P - Q) \frac{Qx_i}{\|Qx_i\|} \right\|^2 = \lambda_i(2 - \lambda_i),$$

and therefore that $\sup_{\theta \in \mathbb{S}_d} \|(P - Q)\theta\|$ is reached on $\mathbf{Im}(Q)$. Finally, if $q = 0$, then $P - Q$ is the null operator, so that $\sup_{\theta \in \mathbb{S}_d} \|(P - Q)\theta\|$ is reached everywhere, including on $\mathbf{Im}(Q) \cap \mathbb{S}_d$. \square

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